1,2-Dibromoethylene

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 13.4 mmHg

Global applicability domain: Inside

Local applicability domain index: 7.70e-01

Confidence level: 6.47e-01

Nearest Neighbors from the Training Set

Image not found
1,4-Difluorobenzene
Measured: 31.0
Predicted: 60.8

Image not found
Trimethyl phosphate
Measured: 7.58
Predicted: 6.80e-01

Image not found
Propyl chloroformate
Measured: 1.36
Predicted: 8.39

Image not found
Linalool
Measured: 7.84
Predicted: 1.06e-01

Image not found
Formic acid, 2-methylpropyl ester
Measured: 13.9
Predicted: 41.0